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Scientific and Technical Information Center

# SEARCH REQUEST FORM

Requester's Full Name: MARK PERCH Examiner #: 59193 Date: 12/2/05  
 Art Unit: 1624 Phone Number: 2- 0663 Serial Number: 1071641  
 Location (Bldg/Room#): 5C01 (Mailbox #): 5C18 Results Format Preferred (circle): PAPER DISK

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: \_\_\_\_\_

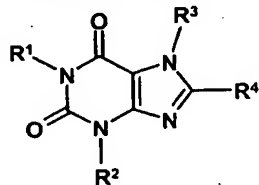
Inventors (please provide full names): \_\_\_\_\_

Earliest Priority Date: \_\_\_\_\_

**Search Topic:**

Search Topic: Search for a new species of the genus *Staphylinus* in the family Staphylinidae, subfamily Staphylininae, tribe Staphylinini, subtribe Staphylinina, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

\* For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional or issued patent numbers) along with the appropriate serial number


$$n_2 = H/C$$

$D_2 = C$ , but  $R_3 \neq CH_3$

$R_4 = -N \begin{array}{c} C_i \\ | \\ C_j-N \end{array}$  or  $-N \begin{array}{c} C_j \\ | \\ C_i-N \end{array}$  or  $\begin{array}{c} C_i \\ | \\ C_j-N \end{array}$  or  $N-C_p-\begin{array}{c} C_j \\ | \\ C_i-N \end{array}$  or  $C_{2-5}-N$

$$R_i = C_n - Q$$

↑  
chain only,  $n = 1-7$

$$Q = \text{G-E-A} \text{ or } \text{C=O-L}$$
$$L = \text{Indole} \text{ or } \text{N-methylindole}$$

$O_n \quad m=2-4 ; \quad j=1-3$

$$E = O/S/N-N/N-O/C-O/C-S^I/C-N \quad p=0-2$$
$$G = \begin{array}{c} \text{O} \\ \parallel \\ \text{C} \end{array} \mid \begin{array}{c} \text{S} \\ \parallel \\ \text{C} \end{array} \mid \begin{array}{c} \text{N} \\ \parallel \\ \text{C} \end{array} \mid \begin{array}{c} \text{C} \\ \parallel \\ \text{C} \end{array} \mid \begin{array}{c} \text{O} \\ \parallel \\ \text{S} \end{array} \quad n=1-2$$
$$A = \text{C}_6\text{H}_5 - \text{C}_5 \text{ or } \text{Hg} - \text{C}_5$$
$$S = 0-7$$

↑ must be unsaturated

**STAFF USE ONLY**

Searcher: \_\_\_\_\_

Searcher Phone #: \_\_\_\_\_

Searcher Location: \_\_\_\_\_

Date Searcher Picked Up: \_\_\_\_\_

Date Completed: \_\_\_\_\_

Searcher Prep & Review Time: \_\_\_\_\_

Online Time: \_\_\_\_\_

### Type of Search

NA Sequence (#)

AA Sequence (#)

\_\_\_\_\_ Structure (#)

### Bibliographic

## Litigation

[Fulltext](#)

Other \_\_\_\_\_

**Vendors and cost where applicable**

STN            Dialog

Questel/Orbit Lexis/Nexis

Westlaw WWW/Internet

### In-house sequence systems

Commercial      Oligomer      Score/Length

☐ Interference      ☐ SPDI      ☐ Encode/Transl

Other (specify) \_\_\_\_\_

# Structure search in REGISTRY (cross to CAPlus, USPatFull)

Berch 10\_716141

12/15/2005

=> file registry

FILE 'REGISTRY' ENTERED AT 16:43:20 ON 15 DEC 2005

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 DEC 2005 HIGHEST RN 869939-98-0

DICTIONARY FILE UPDATES: 14 DEC 2005 HIGHEST RN 869939-98-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
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\*\*\*\*\*

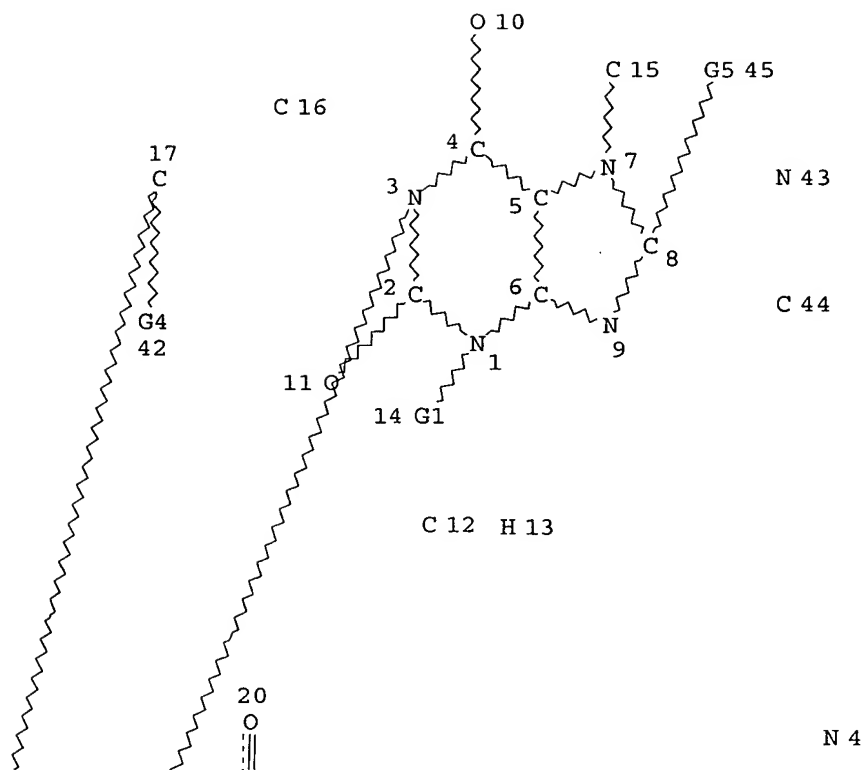
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> d stat que L29

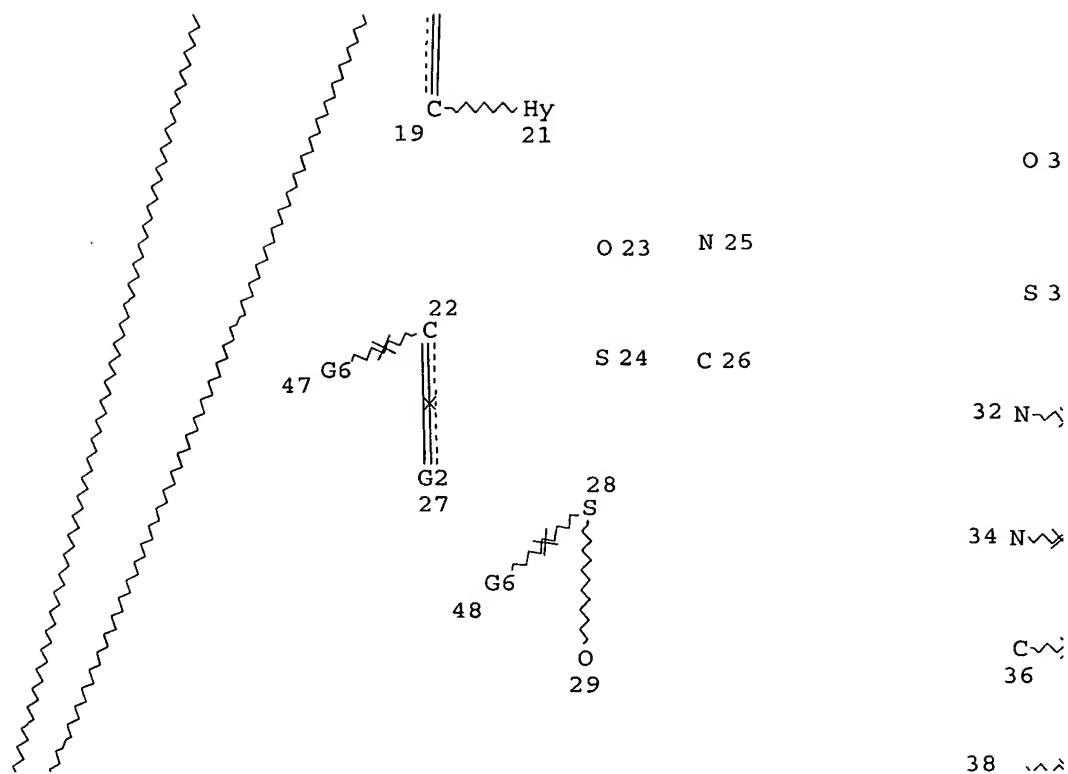
L12 STR



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Page 1-B



Page 2-A  
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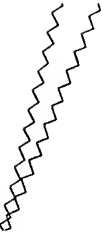
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
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
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△


Page 2-B


18  G20

38 

40 

Page 3-A

 S 39

 N 41

Page 3-B

VAR G1=12/13

VAR G2=23/24/25/26

VAR G4=19/22/28

VAR G5=43/44

VAR G6=30/31/32/34/36/38/40/46

REP G20=(0-6) 16-3 16-17

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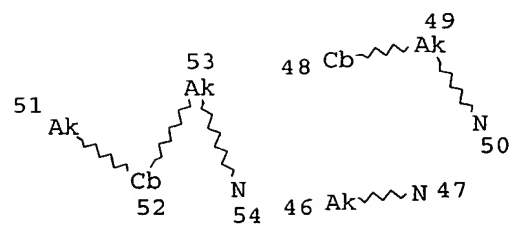
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NSPEC IS RC AT 48  
CONNECT IS E3 RC AT 2  
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CONNECT IS E1 RC AT 10  
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CONNECT IS E1 RC AT 29  
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MLEVEL IS CLASS AT 10 11 12 13 15 16 17 19 20 22 23 24 25 26 28 29 30  
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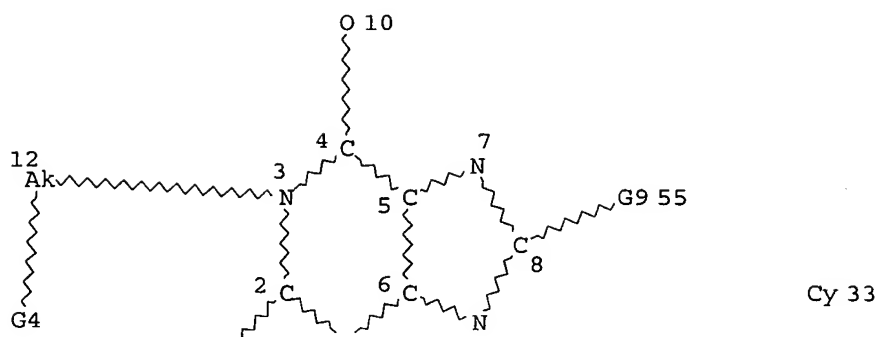
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NUMBER OF NODES IS 48

## STEREO ATTRIBUTES: NONE

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L27 STR



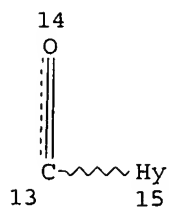
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Page 1-A



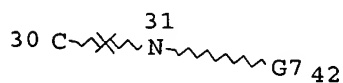
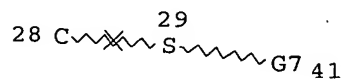
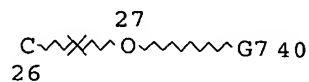
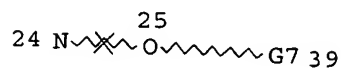
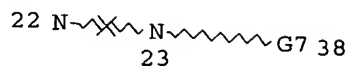
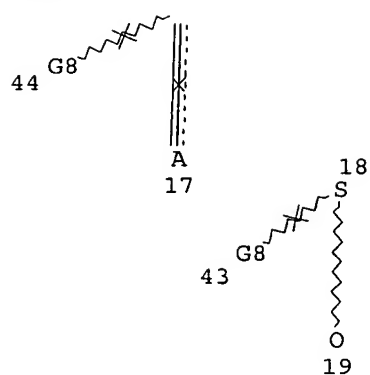
35 Ak ~~~~~ Cy 34



20 O ~~~~~ G7 36

21 S ~~~~~ G7 37

Page 2-A



Page 3-A

VAR G4=13/16/18

VAR G7=33/35

VAR G8=20/21/22/24/26/28/30

VAR G9=45/46/48/51

NODE ATTRIBUTES:

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NSPEC	IS RC	AT	27
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CONNECT IS E3  RC AT   4
CONNECT IS E2  RC AT   9
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DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS AT  10 11 12 13 14 16 17 18 19 20 21 22 23 24 25 26 27
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GGCAT   IS PCY  LOQ  UNS AT  15
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DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M1 N  AT  15

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## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 55

## STEREO ATTRIBUTES: NONE

L29 29 SEA FILE=REGISTRY SUB=L14 SSS FUL L27

100.0% PROCESSED 866 ITERATIONS  
SEARCH TIME: 00.00.01

29 ANSWERS

=&gt; d L34

L34 ANALYZE L29 1- LC : 3 TERMS

TERM # # OCC # DOC % DOC LC

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2      27      27  93.10 CAPLUS
3      17      17  58.62 USPATFULL
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FILE LAST UPDATED: 14 Dec 2005 (20051214/ED)

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=> d que nos L30

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L12      STR
L14      866 SEA FILE=REGISTRY SSS FUL L12
L27      STR
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L30      4 SEA FILE=CAPLUS ABB=ON PLU=ON L29
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=> file uspatfull

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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 15 Dec 2005 (20051215/PD)  
FILE LAST UPDATED: 15 Dec 2005 (20051215/ED)  
HIGHEST GRANTED PATENT NUMBER: US6976271  
HIGHEST APPLICATION PUBLICATION NUMBER: US2005278816  
CA INDEXING IS CURRENT THROUGH 15 Dec 2005 (20051215/UPCA)  
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 15 Dec 2005 (20051215/PD)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2005  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2005

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>>> USPAT2 is now available.  USPATFULL contains full text of the  <<<
>>> original, i.e., the earliest published granted patents or      <<<
>>> applications.  USPAT2 contains full text of the latest US      <<<
>>> publications, starting in 2001, for the inventions covered in  <<<
>>> USPATFULL.  A USPATFULL record contains not only the original  <<<
>>> published document but also a list of any subsequent          <<<
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>>> publications. The publication number, patent kind code, and <<<  
>>> publication date for all the US publications for an invention <<<  
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<  
>>> records and may be searched in standard search fields, e.g., /PN, <<<  
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<  
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<  
>>> enter this cluster. <<<  
>>> <<<  
>>> Use USPATALL when searching terms such as patent assignees, <<<  
>>> classifications, or claims, that may potentially change from <<<  
>>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

=> d que nos L35

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L14 866 SEA FILE=REGISTRY SSS FUL L12  
L27 STR  
L29 29 SEA FILE=REGISTRY SUB=L14 SSS FUL L27  
L35 3 SEA FILE=USPATFULL ABB=ON PLU=ON L29

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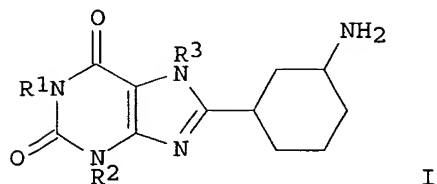
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PROCESSING COMPLETED FOR L30  
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L36 7 DUP REM L30 L35 (0 DUPLICATES REMOVED)  
ANSWERS '1-4' FROM FILE CAPLUS  
ANSWERS '5-7' FROM FILE USPATFULL

=> d ibib abs hitstr L36 1-7

L36 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2004:182879 CAPLUS  
DOCUMENT NUMBER: 140:235743  
TITLE: Preparation of 8-[3-aminopiperidin-1-yl]xanthines as  
dipeptidylpeptidase-IV (DPP-IV) inhibitors.  
INVENTOR(S): Himmelsbach, Frank; Langkopf, Elke; Eckhardt,  
Matthias; Mark, Michael; Maier, Roland; Lotz, Ralf  
Richard Hermann; Tadayyon, Mohammad  
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G.,  
Germany  
SOURCE: PCT Int. Appl., 226 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004018468	A2	20040304	WO 2003-EP9127	20030818
WO 2004018468	A3	20040408		
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CA 2496249	AA	20040304	CA 2003-2496249	20030818
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			DE 2003-10312353	A 20030320
			WO 2003-EP9127	W 20030818
OTHER SOURCE(S):			MARPAT 140:235743	
GI				



AB Title compds. (I; R1 = Me substituted by Me2NCO, pyrrolidin-1-ylcarbonyl, piperidin-1-ylcarbonyl, tert-butylcarbonyl, naphthyl, nitronaphthyl, dimethylaminonaphthyl, phenyloxadiazolyl, quinolinyl, indolyl, cinnolinyl, benzothienyl, etc.; R2 = Me, Me2CH, Ph; R3 = 2-methyl-2-propen-1-yl, 2-chloro-2-propen-1-yl, 3-bromo-2-propen-1-yl, 2-buten-1-yl, 2,3-dimethyl-2-buten-1-yl, 2-butyn-1-yl, 1-cyclopenten-1-ylmethyl, 2-furylmethyl), were prepared Thus, 1,3-dimethyl-7-(2,6-dicyanobenzyl)-8-bromoxanthine (preparation from 8-bromotheophylline and 2-bromomethylisophthalonitrile given), 3-aminopiperidine dihydrochloride, and K2CO3 were heated in DMF for 3 h at 80° to give 14% 1,3-dimethyl-7-(2,6-dicyanobenzyl)-8-(3-aminopiperidin-1-yl)xanthine. I inhibited DPP-IV with IC50 = 1-2160 nM.

IT 668270-29-9P 668270-98-2P 668271-03-2P  
668271-15-6P 668271-65-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

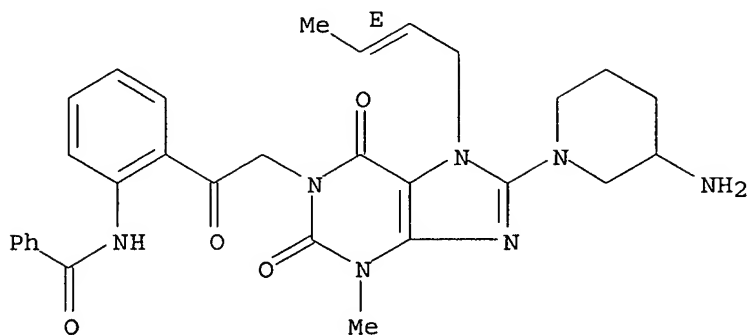
(preparation of aminopiperidinyloxanthines as dipeptidylpeptidase-IV inhibitors)

RN 668270-29-9 CAPLUS

CN Benzamide, N-[2-[[8-(3-amino-1-piperidinyl)-7-(2E)-2-butenyl-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]phenyl]- (9CI) (CA

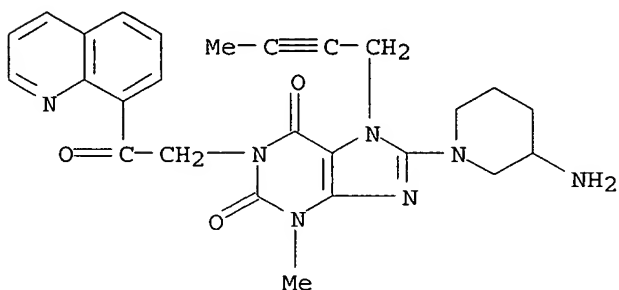
INDEX NAME)

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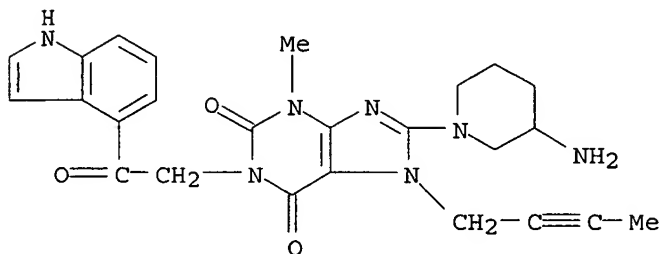
RN 668270-98-2 CAPLUS

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RN 668271-03-2 CAPLUS

CN 1H-Purine-2,6-dione, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-3,7-dihydro-1-[2-(1H-indol-4-yl)-2-oxoethyl]-3-methyl- (9CI) (CA INDEX NAME)



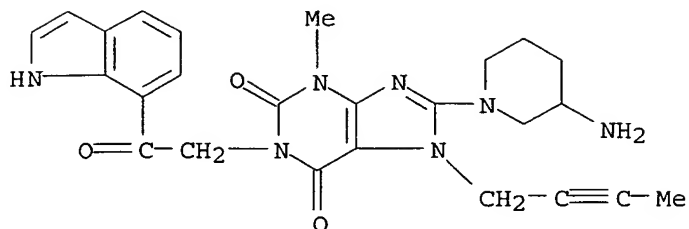
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CM 1

CRN 668271-14-5

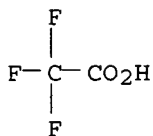
CMF C25 H27 N7 O3



CM 2

CRN 76-05-1

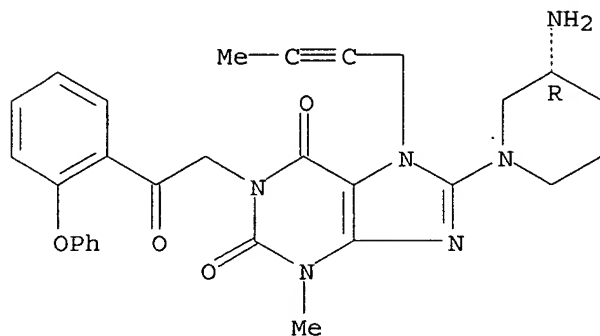
CMF C2 H F3 O2



RN 668271-65-6 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-3,7-dihydro-3-methyl-1-[2-oxo-2-(2-phenoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 668272-79-5P 668273-56-1P 668274-25-7P

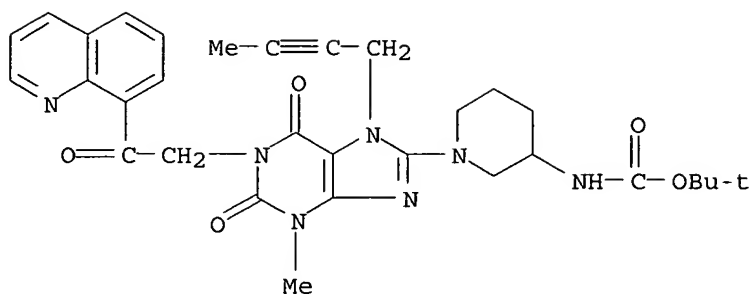
668274-76-8P 668275-19-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aminopiperidinylxanthines as dipeptidylpeptidase-IV inhibitors)

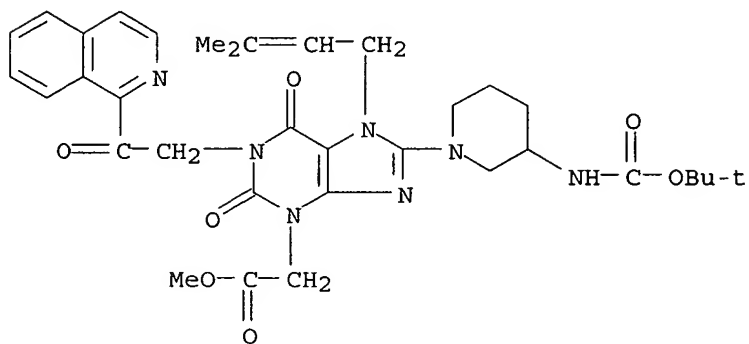
RN 668272-79-5 CAPLUS

CN Carbamic acid, [1-[7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-[2-oxo-2-(8-quinolinyl)ethyl]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



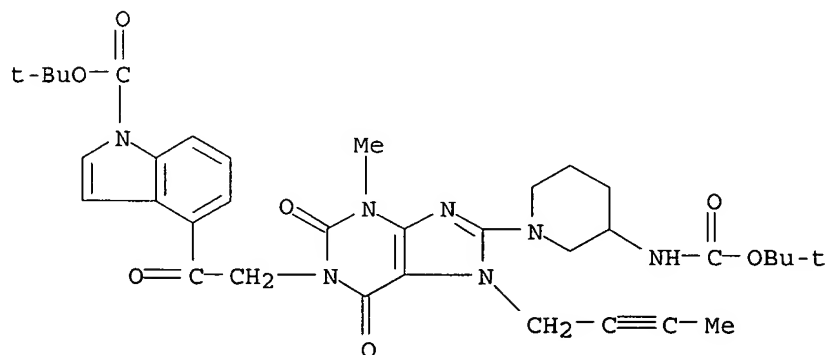
RN 668273-56-1 CAPLUS

CN 3H-Purine-3-acetic acid, 8-[3-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-1,2,6,7-tetrahydro-1-[2-(1-isoquinolinyl)-2-oxoethyl]-7-(3-methyl-2-butenyl)-2,6-dioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 668274-25-7 CAPLUS

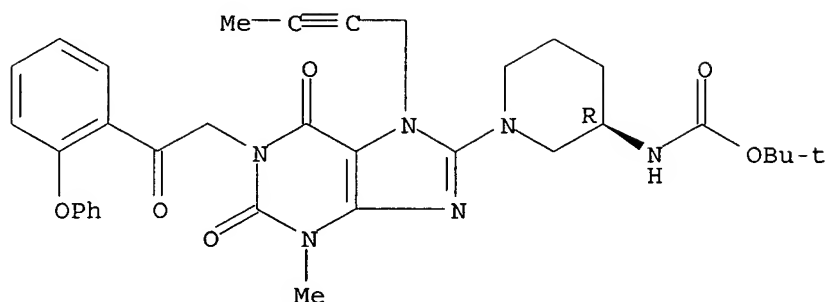
CN 1H-Indole-1-carboxylic acid, 4-[[[7-(2-butynyl)-8-[3-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 668274-76-8 CAPLUS

CN Carbamic acid, [(3R)-1-[7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-[2-oxo-2-(2-phenoxyphenyl)ethyl]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

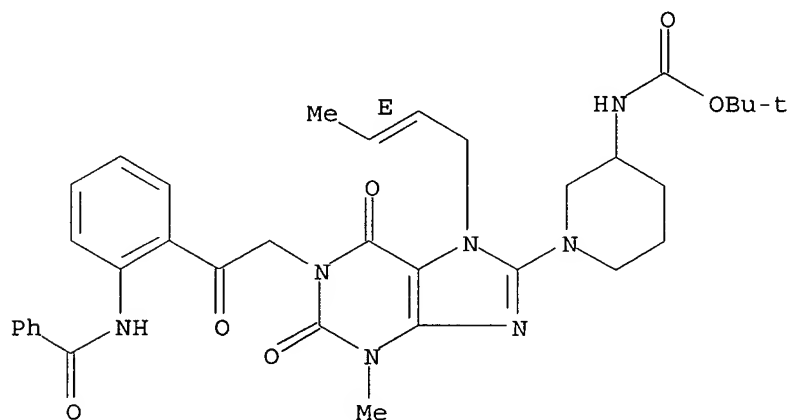
Absolute stereochemistry.



RN 668275-19-2 CAPLUS

CN Carbamic acid, [1-[1-[2-[2-(benzoylamino)phenyl]-2-oxoethyl]-7-(2E)-2-butenyl-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L36 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:450501 CAPLUS

DOCUMENT NUMBER: 141:23542

TITLE: Preparation of xanthine derivatives as dipeptidylpeptidase IV inhibitors

INVENTOR(S): Eckhardt, Matthias; Himmelsbach, Frank; Langkopf, Elke; Maier, Roland; Mark, Michael; Tadayyon, Mohammad  
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. Kg, Germany  
 SOURCE: Ger. Offen., 31 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

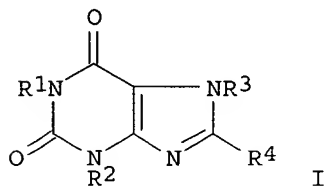
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10254304	A1	20040603	DE 2002-10254304	20021121



WO 2004046148 A1 20040603 WO 2003-EP12821 20031111  
 WO 2004046148 C1 20050714  
 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 EP 1565468 A1 20050824 EP 2003-782204 20031111  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 CA 2506720 AA 20040603 CA 2003-2506720 20031117  
 US 2004138215 A1 20040715 US 2003-716141 20031118  
 PRIORITY APPLN. INFO.: DE 2002-10254304 A 20021121  
 US 2002-432450P P 20021211  
 WO 2003-EP12821 W 20031111  
 OTHER SOURCE(S): MARPAT 141:23542  
 GI



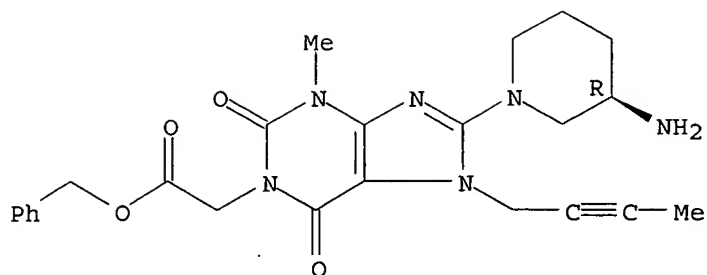
AB Title compds. [I; R1 = ABD; A = (substituted) alkyl, etc.; B = EG; E = O, S, etc.; G = (thio)carbonyl, (imino-substituted) Me, etc.; D = propionyl, (fluorinated) alkyl, alkenyl; R2 = H, alkyl, alkenyl, alkynyl, cycloalkyl, etc.; R3 = (substituted) alkyl, aryl, furanyl, thienyl, oxazolyl, isoxazolyl, etc.; R4 = (substituted) azetidin-1-yl, pyrrolidin-1-yl, piperidin-1-yl, etc.], were prepared Thus, 1-[(benzyloxycarbonyl)methyl]-3-methyl-7-(2-butyn-1-yl)-8[(R)-3-(tert-butyloxycarbonylamino)piperidin-1-yl]xanthine (preparation given) in CH<sub>2</sub>Cl<sub>2</sub> was shaken with CF<sub>3</sub>CO<sub>2</sub>H for 20 min at 30° to give 97% 1-[(benzyloxycarbonyl)methyl]-3-methyl-7-(2-butyn-1-yl)-8[(R)-3-aminopiperidin-1-yl]xanthine. The latter inhibited dipeptidylpeptidase IV (DPP IV) with IC<sub>50</sub> = 27 nM.

IT 697806-80-7P 697806-84-1P 697806-90-9P  
 697806-92-1P 697806-93-2P 697806-95-4P  
 697806-96-5P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of xanthine derivs. as dipeptidylpeptidase IV inhibitors)

RN 697806-80-7 CAPLUS

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

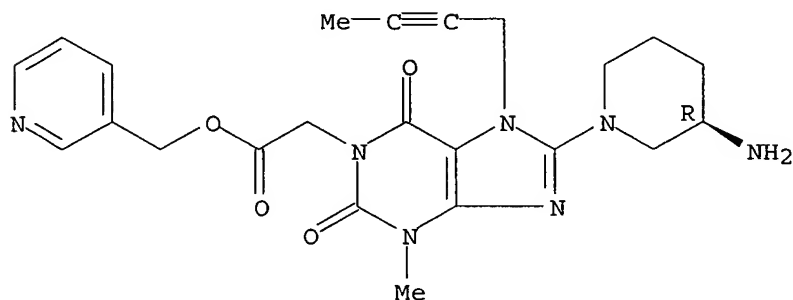
Absolute stereochemistry.



RN 697806-84-1 CAPLUS

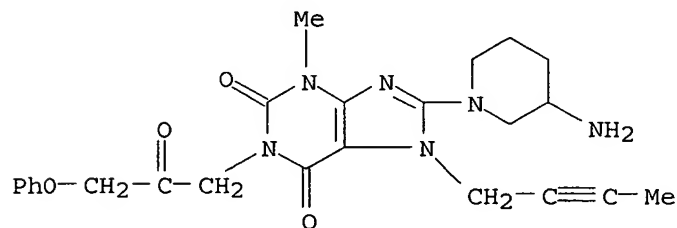
CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, 3-pyridinylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 697806-90-9 CAPLUS

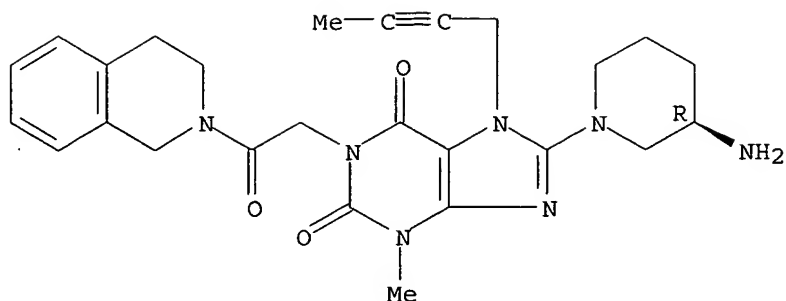
CN 1H-Purine-2,6-dione, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-3,7-dihydro-3-methyl-1-(2-oxo-3-phenoxypropyl)- (9CI) (CA INDEX NAME)



RN 697806-92-1 CAPLUS

CN Isoquinoline, 2-[[8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

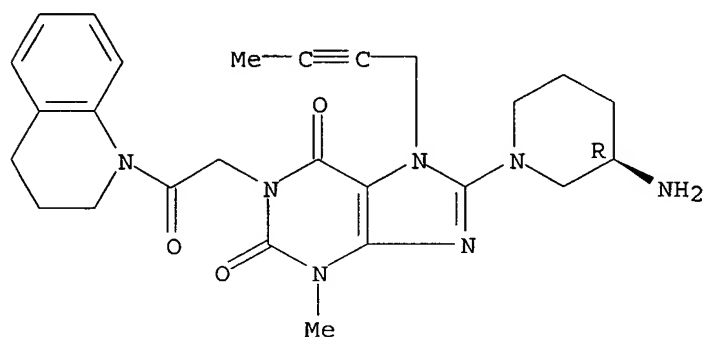
Absolute stereochemistry.



RN 697806-93-2 CAPLUS

CN Quinoline, 1-[[8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-1,2,3,4-tetrahydro-(9CI) (CA INDEX NAME)

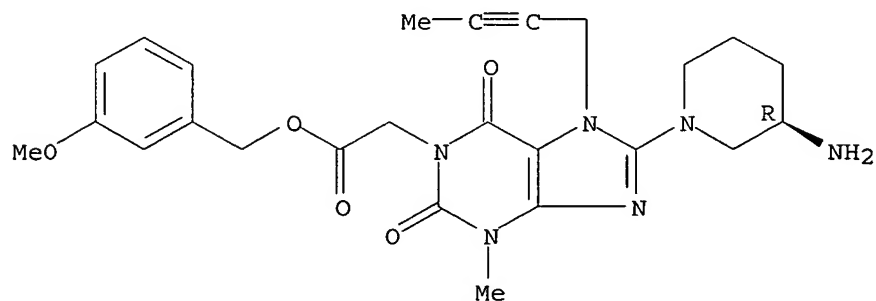
Absolute stereochemistry.



RN 697806-95-4 CAPLUS

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

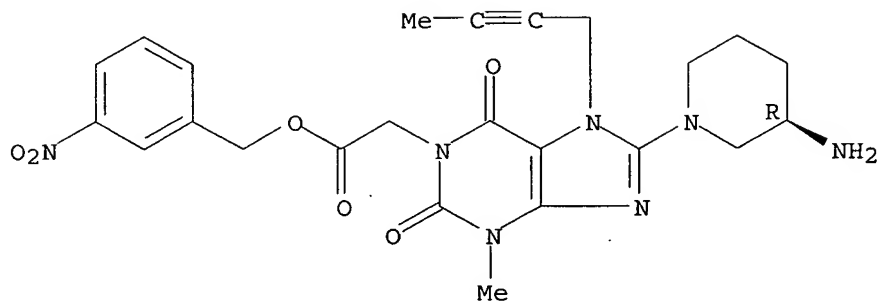
Absolute stereochemistry.



RN 697806-96-5 CAPLUS

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 697806-55-6P 697806-59-0P 697806-67-0P  
697806-68-1P 697806-72-7P 697806-75-0P  
697806-76-1P

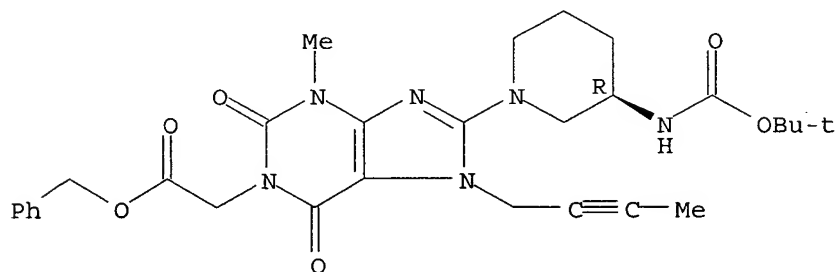
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation of xanthine derivs. as dipeptidylpeptidase IV inhibitors)

RN 697806-55-6 CAPLUS

CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

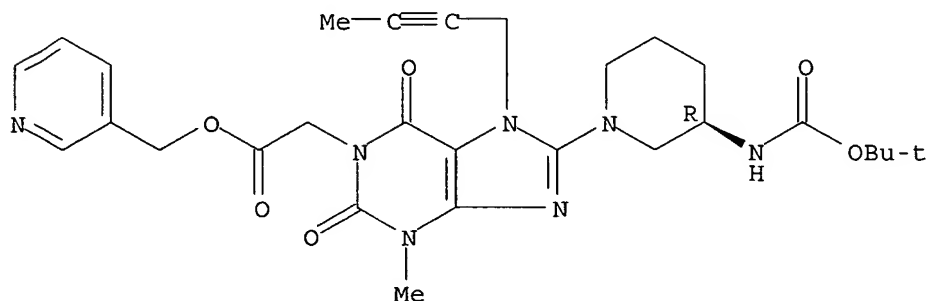
Absolute stereochemistry.



RN 697806-59-0 CAPLUS

CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, 3-pyridinylmethyl ester (9CI) (CA INDEX NAME)

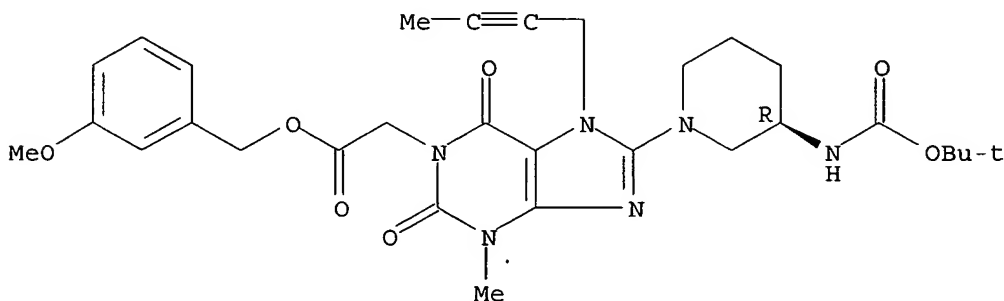
Absolute stereochemistry.



RN 697806-67-0 CAPLUS

CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

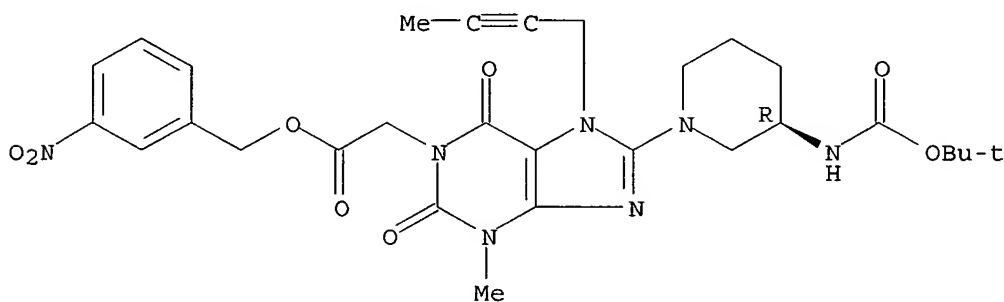
Absolute stereochemistry.



RN 697806-68-1 CAPLUS

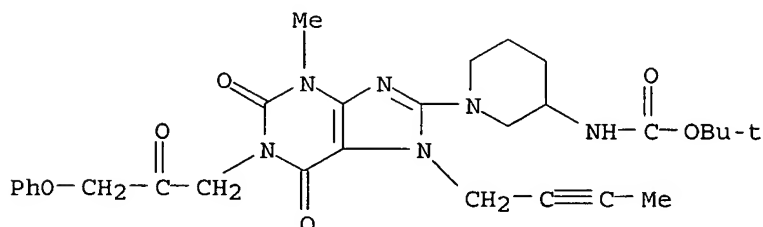
CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 697806-72-7 CAPLUS

CN Carbamic acid, [1-[7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-3-phenoxypropyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

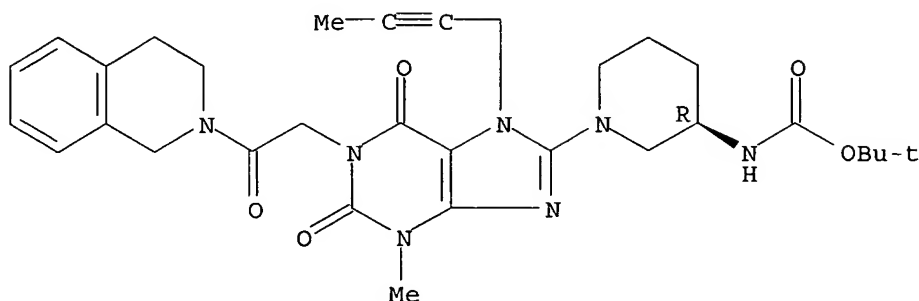


RN 697806-75-0 CAPLUS

CN Carbamic acid, [(3R)-1-[7-(2-butynyl)-1-[2-(3,4-dihydro-2(1H)-isoquinolinyl)-2-oxoethyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-

8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

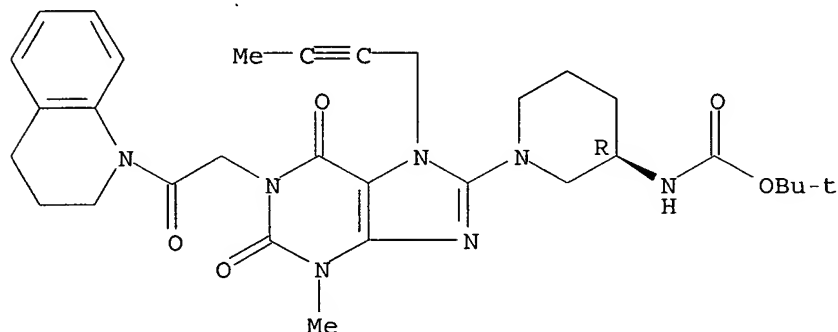
Absolute stereochemistry.



RN 697806-76-1 CAPLUS

CN Carbamic acid, [(3R)-1-[7-(2-butynyl)-1-[2-(3,4-dihydro-1(2H)-quinolinyl)-2-oxoethyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L36 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:177908 CAPLUS

DOCUMENT NUMBER: 140:235733

TITLE: Preparation of xanthines as dipeptidylpeptidase IV inhibitors for the treatment of diabetes

INVENTOR(S): Eckhardt, Matthias; Himmelsbach, Frank; Langkopf, Elke; Maier, Roland; Mark, Michael; Lotz, Ralf

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G., Germany

SOURCE: Ger. Offen., 22 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10238470	A1	20040304	DE 2002-10238470	20020822
US 2004166125	A1	20040826	US 2003-636088	20030807

CA 2496325 AA 20040304 CA 2003-2496325 20030816  
 WO 2004018467 A2 20040304 WO 2003-EP9096 20030816  
 WO 2004018467 A3 20040513

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

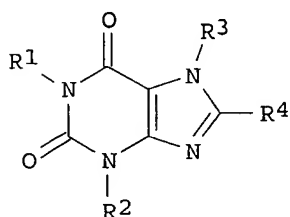
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EP 1554278 A2 20050720 EP 2003-792342 20030816

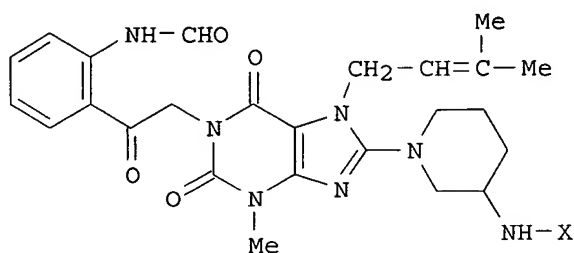
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PRIORITY APPLN. INFO.: DE 2002-10238470 A 20020822  
 US 2002-409258P P 20020909  
 WO 2003-EP9096 W 20030816

OTHER SOURCE(S): MARPAT 140:235733  
 GI



I



II

AB Title compds. I [R1 = (un)substituted phenylcarbonylmethyl; R2 = H, alkyl, alkenyl, etc.; R3 = (un)substituted alkyl; R4 = (un)substituted azetidin-1-yl, pyrrolidin-1-yl] and their pharmaceutically acceptable salts were prepared. For example, BOC deprotection of amine II (X = Boc), e.g., prepared from 3-Methyl-8-chloroxanthine, via TFA afforded claimed xanthine II (X = H) in 87% yield. In dipeptidylpeptidase IV inhibition assays, 7-examples of compds. I exhibited IC50 values ranging from 3-11 nM, e.g., the IC50 value of xanthine II (X = H) was 5 nM. Compds. I are claimed useful for the treatment of type I and type II diabetes.

IT 666816-82-6P

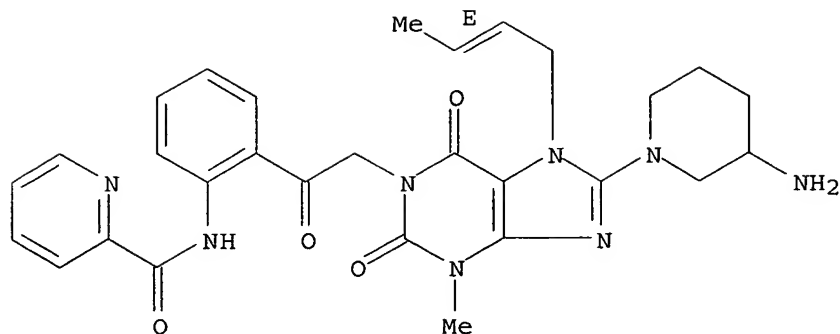
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of xanthines as dipeptidylpeptidase IV inhibitors for the treatment of diabetes)

RN 666816-82-6 CAPLUS

CN 2-Pyridinecarboxamide, N-[2-[[8-(3-amino-1-piperidinyl)-7-(2E)-2-butenyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT 666817-05-6P

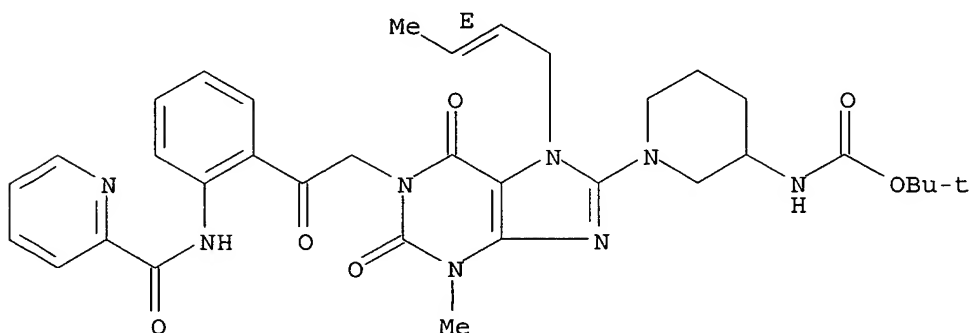
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of xanthines as dipeptidylpeptidase IV inhibitors for the treatment of diabetes)

RN 666817-05-6 CAPLUS

CN Carbamic acid, [1-[7-(2E)-2-butenyl-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-[2-oxo-2-[2-[(2-pyridinylcarbonyl)amino]phenyl]ethyl]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L36 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:675555 CAPLUS

DOCUMENT NUMBER: 139:197299

TITLE: Preparation of xanthine derivatives as DPP-IV inhibitors

INVENTOR(S): Yoshikawa, Seiji; Emori, Eita; Matsuura, Fumiyoshi; Clark, Richard; Ikuta, Hironori; Yasuda, Nobuyuki; Nagakura, Tadashi; Yamazaki, Kazuto; Aoki, Mika

PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 217 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

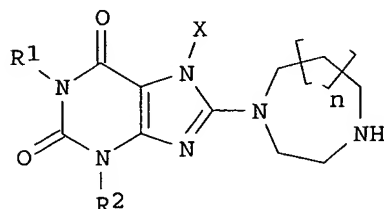
FAMILY ACC. NUM. COUNT: 1

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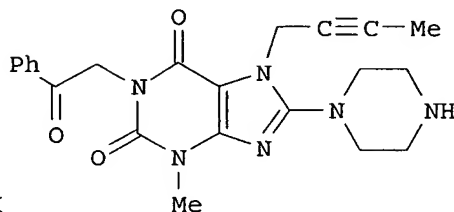
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 1338595 A2 20030827 EP 2003-290431 20030224  
 EP 1338595 A3 20031008  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 JP 2004043429 A2 20040212 JP 2003-44771 20030221  
 US 2004082570 A1 20040429 US 2003-374918 20030224  
 PRIORITY APPLN. INFO.: JP 2002-47761 A 20020225  
 JP 2002-149557 A 20020523  
 OTHER SOURCE(S): MARPAT 139:197299  
 GI



I



II

AB Novel xanthine derivs. of formula I [R1, R2 = H, alkyl, alkoxy, hydroxyalkyl, cycloalkyl, aryl, etc.; X = alkynyl, (substituted) Ph; n = 0, 1] are prepared which exhibit an excellent dipeptidyl peptidase IV (DPPIV) inhibition effect. Thus, II was prepared, and inhibited DPPIV with IC50 of 0.654 nM, and improved glucose tolerance in mice by 49.4%.

IT 586402-89-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of xanthine derivs. as DPPIV inhibitors)

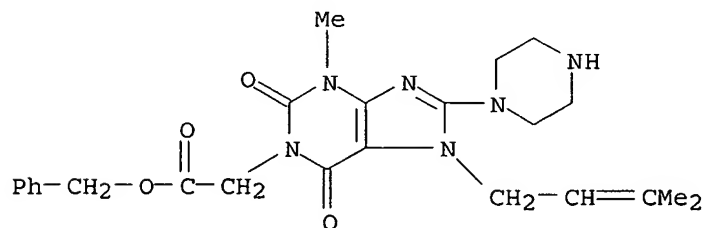
RN 586402-89-3 CAPLUS

CN 1H-Purine-1-acetic acid, 2,3,6,7-tetrahydro-3-methyl-7-(3-methyl-2-butenyl)-2,6-dioxo-8-(1-piperazinyl)-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 586402-88-2

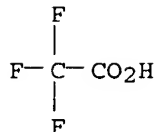
CMF C24 H30 N6 O4



CM 2

CRN 76-05-1

CMF C2 H F3 O2



L36 ANSWER 5 OF 7 USPATFULL on STN

ACCESSION NUMBER: 2004:215019 USPATFULL

TITLE: Xanthine derivatives, their preparation and their use in pharmaceutical compositions

INVENTOR(S): Himmelsbach, Frank, Mittelbiberach, GERMANY, FEDERAL REPUBLIC OF  
 Langkopf, Elke, Warthausen, GERMANY, FEDERAL REPUBLIC OF  
 Eckhardt, Matthias, Biberach, GERMANY, FEDERAL REPUBLIC OF  
 Mark, Michael, Biberach, GERMANY, FEDERAL REPUBLIC OF  
 Maier, Roland, Biberach an der Riss, GERMANY, FEDERAL REPUBLIC OF  
 Lotz, Ralf R. H., Schemmerhofen, GERMANY, FEDERAL REPUBLIC OF

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. KG, Ingelheim, GERMANY, FEDERAL REPUBLIC OF (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004166125	A1	20040826
APPLICATION INFO.:	US 2003-636088	A1	20030807 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	DE 2002-DE10238470	20020822
	US 2002-409258P	20020909 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	BOEHRINGER INGELHEIM CORPORATION, 900 RIDGEBURY ROAD, P. O. BOX 368, RIDGEFIELD, CT, 06877	
NUMBER OF CLAIMS:	15	
EXEMPLARY CLAIM:	1	
LINE COUNT:	1596	
CAS INDEXING IS AVAILABLE FOR THIS PATENT.		
AB	Compounds of formula (I) ##STR1##	

wherein R.sup.1 to R.sup.4 are defined as in the claims, or the prodrugs or salts thereof, particularly the physiologically acceptable salts thereof, pharmaceutical compositions containing these compounds, and methods of treating type I and type II diabetes mellitus, arthritis, obesity, allograft transplantation, or calcitonin-induced osteoporosis using these compounds.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

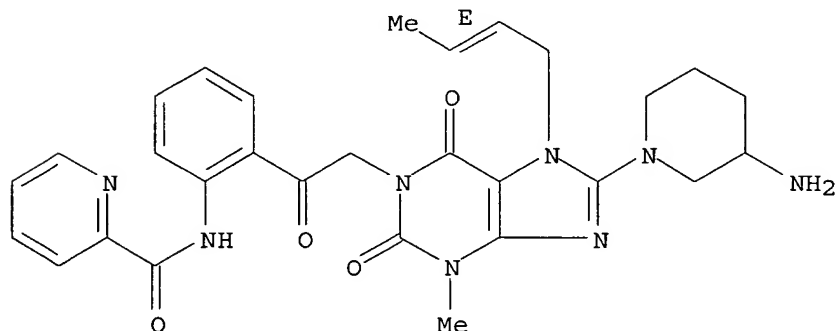
IT 666816-82-6P

(preparation of xanthines as dipeptidylpeptidase IV inhibitors for the treatment of diabetes)

RN 666816-82-6 USPATFULL

CN 2-Pyridinecarboxamide, N-[2-[[8-(3-amino-1-piperidinyl)-7-(2E)-2-butenyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



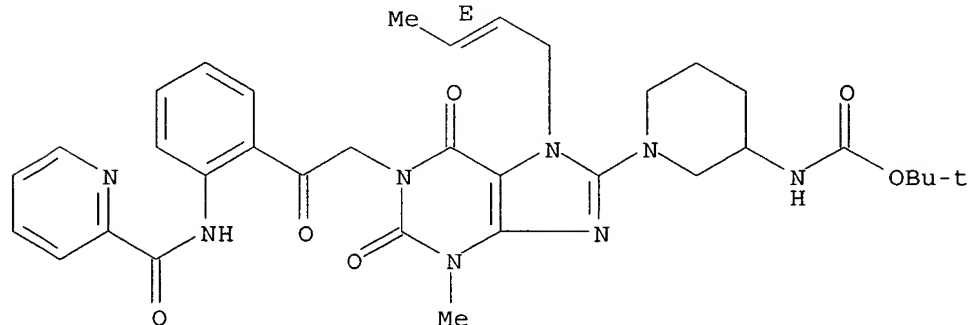
IT 666817-05-6P

(preparation of xanthines as dipeptidylpeptidase IV inhibitors for the treatment of diabetes)

RN 666817-05-6 USPATFULL

CN Carbamic acid, [1-[7-(2E)-2-butenyl-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-[2-oxo-2-[2-[(2-pyridinylcarbonyl)amino]phenyl]ethyl]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L36 ANSWER 6 OF 7 USPATFULL on STN

ACCESSION NUMBER: 2004:179045 USPATFULL

TITLE: Xanthine derivatives, the preparation thereof and their use as pharmaceutical compositions

INVENTOR(S): Eckhardt, Matthias, Biberach, GERMANY, FEDERAL REPUBLIC OF  
Himmelsbach, Frank, Mittelbiberach, GERMANY, FEDERAL REPUBLIC OF  
Langkopf, Elke, Warthausen, GERMANY, FEDERAL REPUBLIC OF

Maier, Roland, Biberach, GERMANY, FEDERAL REPUBLIC OF  
Mark, Michael, Biberach, GERMANY, FEDERAL REPUBLIC OF  
Tadayyon, Mohammad, Ulm, GERMANY, FEDERAL REPUBLIC OF  
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. KG, Ingelheim,

GERMANY, FEDERAL REPUBLIC OF (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004138215	A1	20040715
APPLICATION INFO.:	US 2003-716141	A1	20031118 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	DE 2002-10254304	20021121
	US 2002-432450P	20021211 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	BOEHRINGER INGELHEIM CORPORATION, 900 RIDGEBURY ROAD, P. O. BOX 368, RIDGEFIELD, CT, 06877	
NUMBER OF CLAIMS:	15	
EXEMPLARY CLAIM:	1	
LINE COUNT:	2236	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention relates to substituted xanthenes of general formula ##STR1##

the tautomers, the stereoisomers, the mixtures thereof, the prodrugs thereof and the salts thereof, which have valuable pharmacological properties, particularly an inhibitory effect on the activity of the enzyme dipeptidylpeptidase-IV (DPP-IV).

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

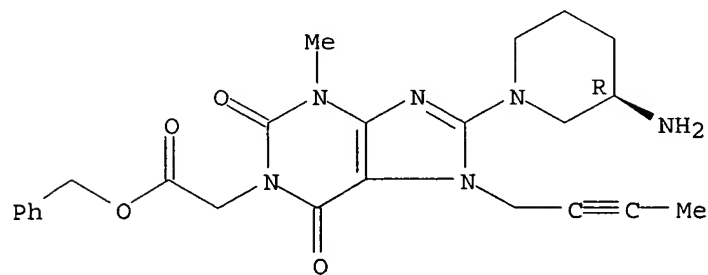
IT 697806-80-7P 697806-84-1P 697806-90-9P  
697806-92-1P 697806-93-2P 697806-95-4P  
697806-96-5P

(preparation of xanthine derivs. as dipeptidylpeptidase IV inhibitors)

RN 697806-80-7 USPATFULL

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-  
2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, phenylmethyl ester (9CI) (CA  
INDEX NAME)

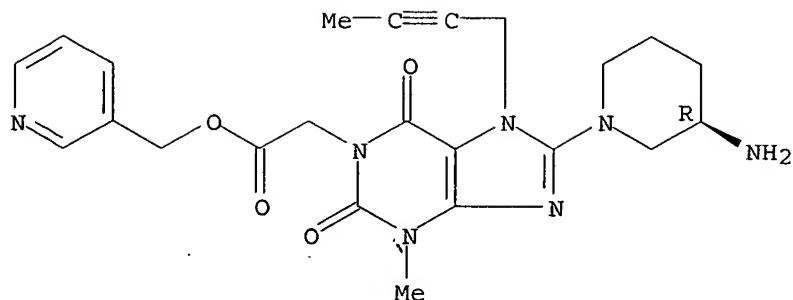
Absolute stereochemistry.



RN 697806-84-1 USPATFULL

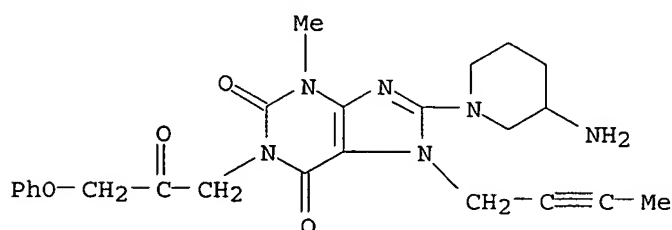
CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-  
2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, 3-pyridinylmethyl ester (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



RN 697806-90-9 USPATFULL

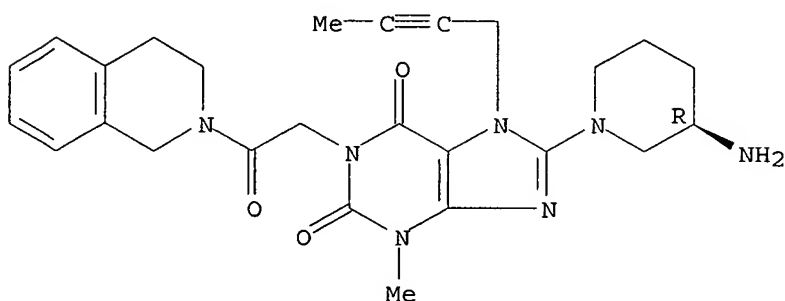
CN 1H-Purine-2,6-dione, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-3,7-dihydro-3-methyl-1-(2-oxo-3-phenoxypropyl)- (9CI) (CA INDEX NAME)



RN 697806-92-1 USPATFULL

CN Isoquinoline, 2-[[8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

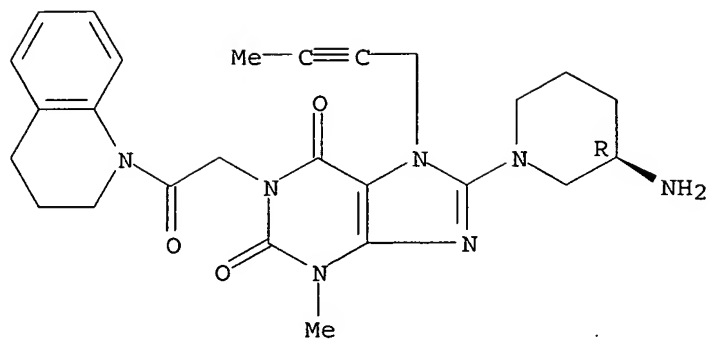
Absolute stereochemistry.



RN 697806-93-2 USPATFULL

CN Quinoline, 1-[[8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

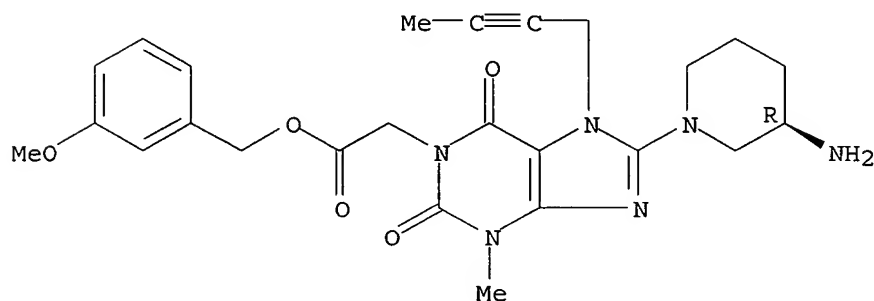
Absolute stereochemistry.



RN 697806-95-4 USPATFULL

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

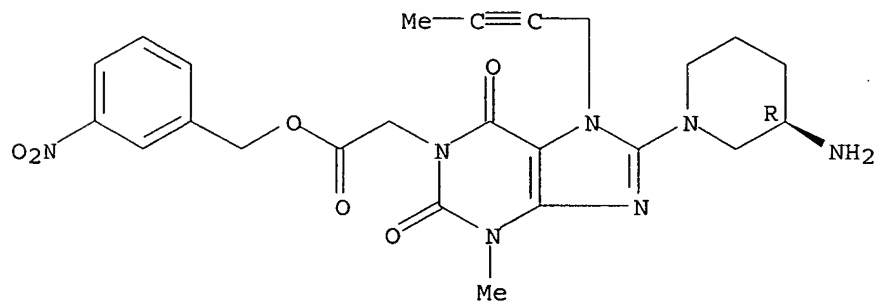
Absolute stereochemistry.



RN 697806-96-5 USPATFULL

CN 1H-Purine-1-acetic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 697806-55-6P 697806-59-0P 697806-67-0P

697806-68-1P 697806-72-7P 697806-75-0P

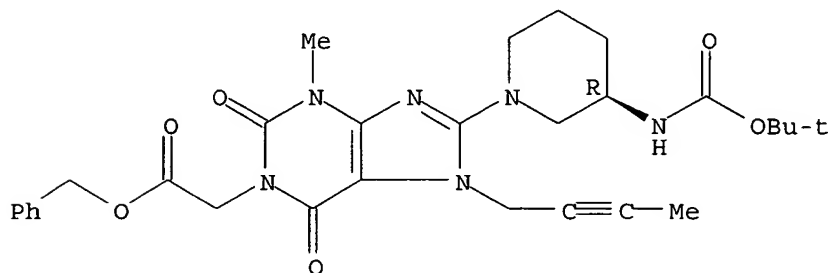
697806-76-1P

(preparation of xanthine derivs. as dipeptidylpeptidase IV inhibitors)

RN 697806-55-6 USPATFULL

CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

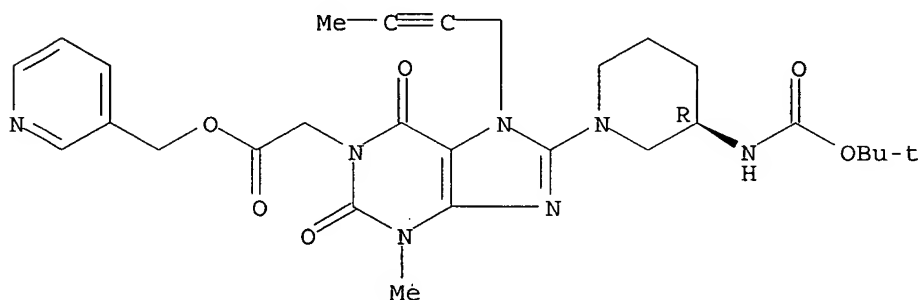
Absolute stereochemistry.



RN 697806-59-0 USPATFULL

CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, 3-pyridinylmethyl ester (9CI) (CA INDEX NAME)

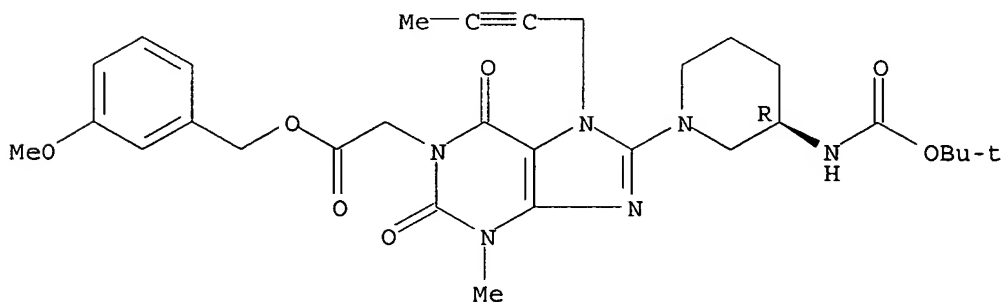
Absolute stereochemistry.



RN 697806-67-0 USPATFULL

CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)

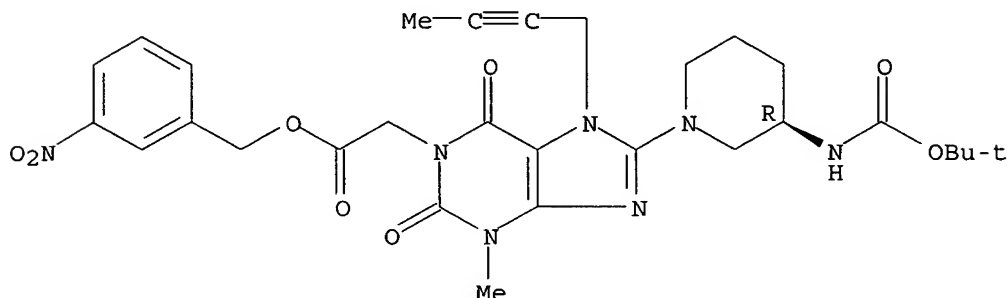
Absolute stereochemistry.



RN 697806-68-1 USPATFULL

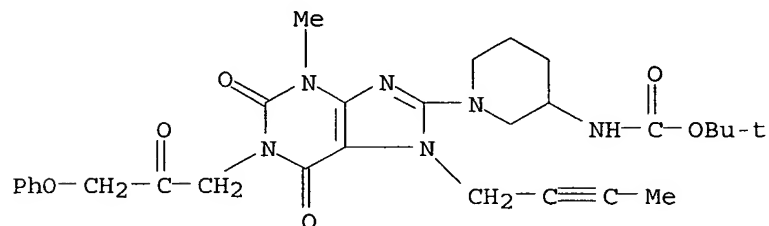
CN 1H-Purine-1-acetic acid, 7-(2-butynyl)-8-[(3R)-3-[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, (3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 697806-72-7 USPATFULL

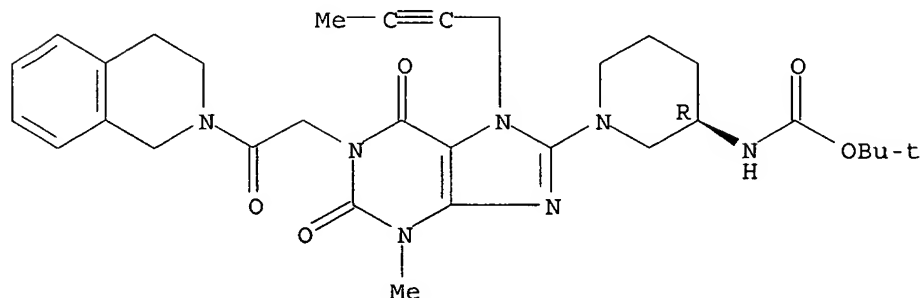
CN Carbamic acid, [1-[7-(2-butynyl)-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-3-phenoxypropyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 697806-75-0 USPATFULL

CN Carbamic acid, [(3R)-1-[7-(2-butynyl)-1-[2-(3,4-dihydro-2(1H)-isoquinolinyl)-2-oxoethyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



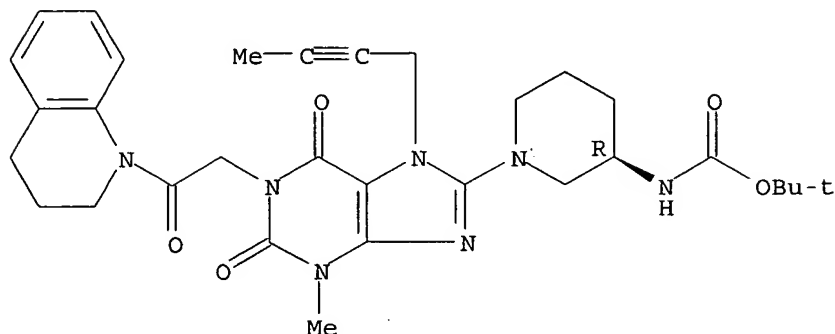
RN 697806-76-1 USPATFULL

CN Carbamic acid, [(3R)-1-[7-(2-butynyl)-1-[2-(3,4-dihydro-1(2H)-quinolinyl)-2-oxoethyl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-8-yl]-3-



piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L36 ANSWER 7 OF 7 USPATFULL on STN

ACCESSION NUMBER: 2004:108168 USPATFULL

TITLE: Xanthine derivative and DPPIV inhibitor

INVENTOR(S): Yoshikawa, Seiji, Ibaraki, JAPAN

Emori, Eita, Ibaraki, JAPAN

Matsuura, Fumiyoshi, Ibaraki, JAPAN

Clark, Richard, Ibaraki, JAPAN

Ikuta, Hironori, Ibaraki, JAPAN

Yasuda, Nobuyuki, Ibaraki, JAPAN

Nagakura, Tadashi, Ibaraki, JAPAN

Yamazaki, Kazuto, Ibaraki, JAPAN

Aoki, Mika, Ibaraki, JAPAN

PATENT ASSIGNEE(S): Eisai Co., Ltd., Tokyo, JAPAN, 112-8088 (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004082570	A1	20040429
APPLICATION INFO.:	US 2003-374918	A1	20030224 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	JP 2002-47761	20020225
	JP 2002-149557	20020523
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	TOWNSEND AND TOWNSEND AND CREW, LLP, TWO EMBARCADERO CENTER, EIGHTH FLOOR, SAN FRANCISCO, CA, 94111-3834	
NUMBER OF CLAIMS:	27	
EXEMPLARY CLAIM:	1	
LINE COUNT:	7402	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides novel compounds exhibiting an excellent DPPIV inhibition effect.

The compounds are represented by the formula: ##STR1##

wherein, m is 0 or 1;

n is 0;

R.sup.31, R.sup.32, R.sup.33, R.sup.34, R.sup.35, R.sup.36, R.sup.37, R.sup.38, R.sup.39, R.sup.40, R.sup.41, and R.sup.42 each represent a hydrogen atom;

X represents an alkynyl group, an aryl group, and such, which group may be substituted; and,

R.sup.1 and R.sup.2 each independently represents a hydrogen atom, an alkyl group, an alkoxy group, or such,

or salts or hydrates thereof.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 586402-89-3P

(preparation of xanthine derivs. as DPPIV inhibitors)

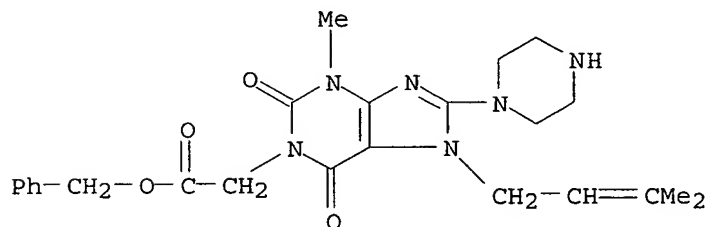
RN 586402-89-3 USPTAFULL

CN 1H-Purine-1-acetic acid, 2,3,6,7-tetrahydro-3-methyl-7-(3-methyl-2-butenyl)-2,6-dioxo-8-(1-piperazinyl)-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 586402-88-2

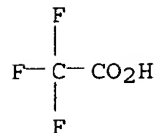
CMF C24 H30 N6 O4



CM 2

CRN 76-05-1

CMF C2 H F3 O2



# Structure search in BEILSTEIN

Berch 10\_716141

12/15/2005

> file beilstein

FILE 'BEILSTEIN' ENTERED AT 16:46:16 ON 15 DEC 2005

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FILE LAST UPDATED ON OCTOBER 10, 2005

FILE COVERS 1771 TO 2005.

\*\*\* FILE CONTAINS 9,363,954 SUBSTANCES \*\*\*

>>>PLEASE NOTE: Reaction Data and substance data are stored in  
separate documents and can not be searched together in one query.  
Reaction data for BEILSTEIN compounds may be displayed  
immediately with the display codes PRE (preparations) and REA  
(reactions). A substance answer set retrieved after the search  
for a chemical name, a compounds with available reaction  
information by combining with PRE/FA, REA/FA or more generally  
with RX/FA. The BEILSTEIN Registry Number (BRN) is the link  
between a BEILSTEIN compound and belonging reactions. For mo  
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>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

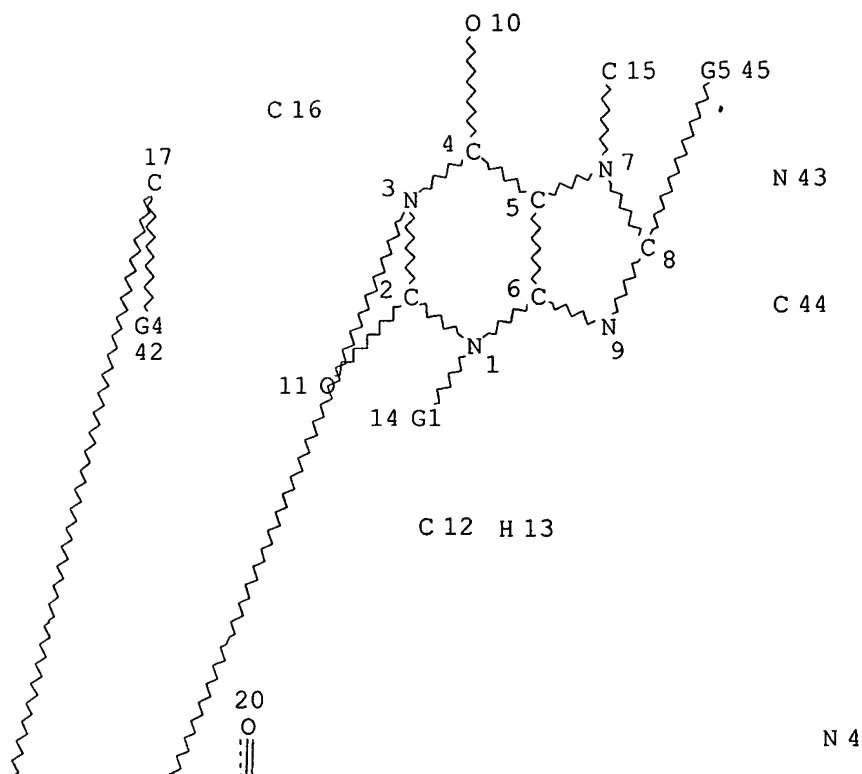
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\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
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## NEW

\* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE  
SEARCHED, SELECTED AND TRANSFERRED.  
\* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,  
ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A  
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=> d stat que L33

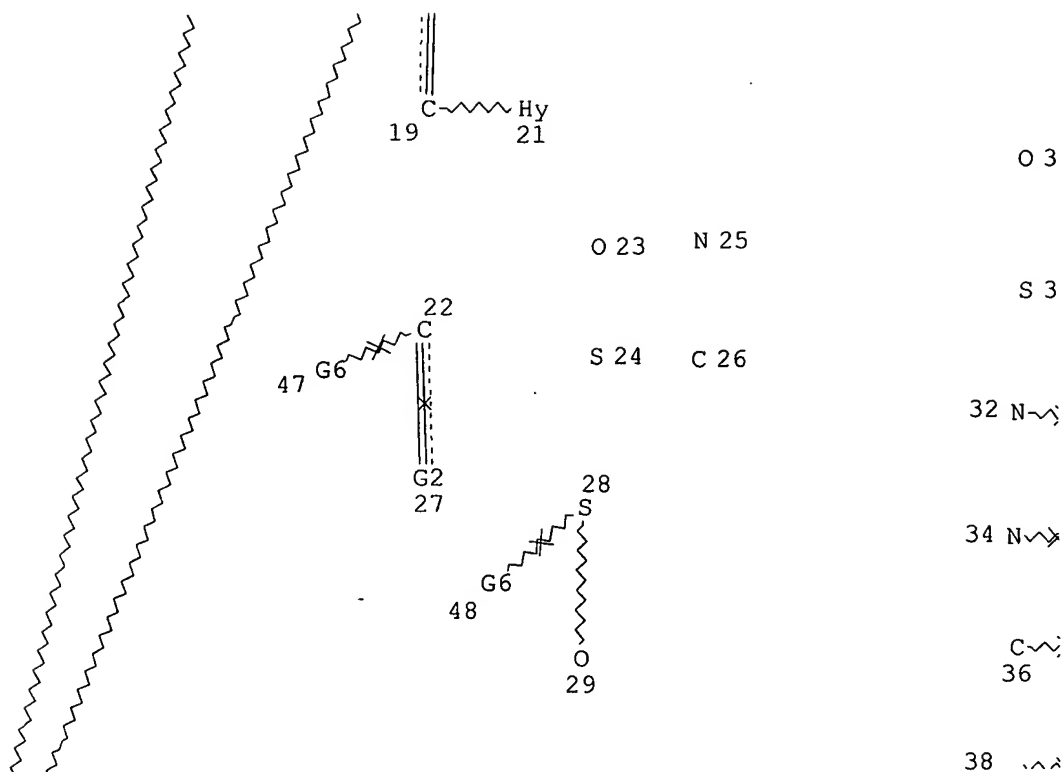
L12 STR



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6

Page 1-B



Page 2-A  
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31

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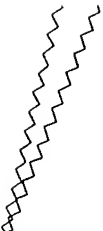
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Page 2-B

18  
G20



38 C~&gt;

40 C~&gt;

Page 3-A

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Page 3-B

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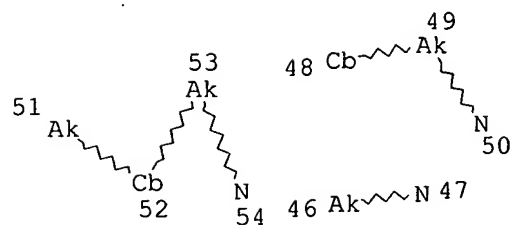
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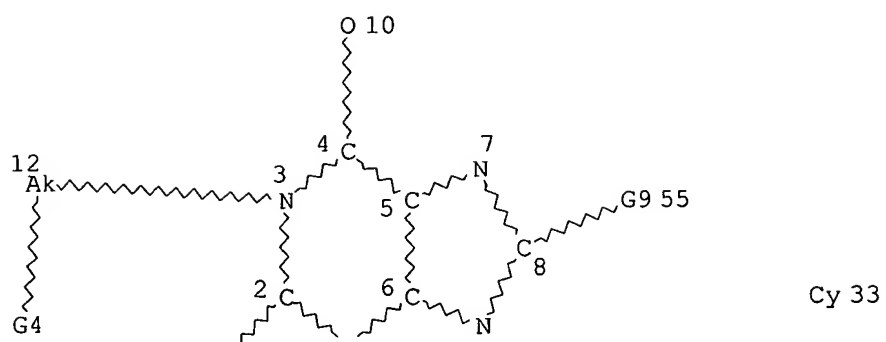
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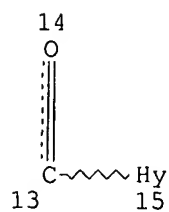
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Page 1-A



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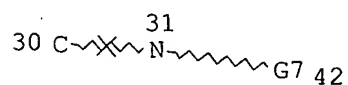
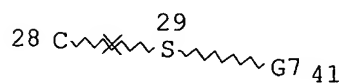
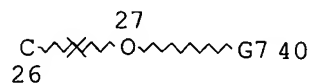
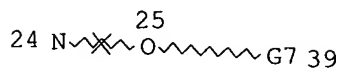
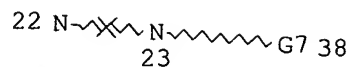
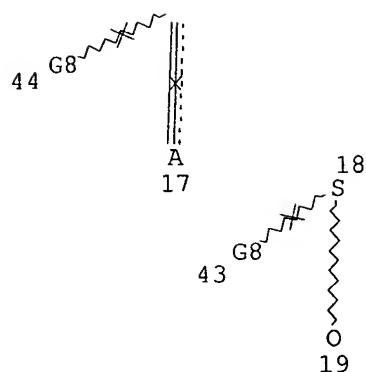
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21 S ~~~~~ G7 37



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Page 3-A

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VAR G9=45/46/48/51

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NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS C	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12
NSPEC	IS C	AT	13
NSPEC	IS C	AT	14
NSPEC	IS C	AT	15
NSPEC	IS RC	AT	16
NSPEC	IS RC	AT	17
NSPEC	IS RC	AT	18
NSPEC	IS C	AT	19
NSPEC	IS RC	AT	20
NSPEC	IS RC	AT	21
NSPEC	IS RC	AT	22
NSPEC	IS RC	AT	23
NSPEC	IS RC	AT	24
NSPEC	IS RC	AT	25
NSPEC	IS RC	AT	26
NSPEC	IS RC	AT	27
NSPEC	IS RC	AT	28

```

NSPEC  IS RC      AT  29
NSPEC  IS RC      AT  30
NSPEC  IS RC      AT  31
NSPEC  IS C       AT  32
NSPEC  IS C       AT  33
NSPEC  IS C       AT  34
NSPEC  IS C       AT  35
NSPEC  IS C       AT  36
NSPEC  IS C       AT  37
NSPEC  IS C       AT  38
NSPEC  IS C       AT  39
NSPEC  IS C       AT  40
NSPEC  IS C       AT  41
NSPEC  IS C       AT  42
NSPEC  IS RC      AT  43
NSPEC  IS RC      AT  44
NSPEC  IS RC      AT  45
NSPEC  IS C       AT  46
NSPEC  IS RC      AT  47
NSPEC  IS C       AT  48
NSPEC  IS C       AT  49
NSPEC  IS RC      AT  50
NSPEC  IS C       AT  51
NSPEC  IS C       AT  52
NSPEC  IS C       AT  53
NSPEC  IS RC      AT  54
NSPEC  IS C       AT  55
CONNECT IS E3  RC AT   2
CONNECT IS E3  RC AT   4
CONNECT IS E2  RC AT   9
CONNECT IS E1  RC AT  10
CONNECT IS E1  RC AT  11
CONNECT IS E1  RC AT  19
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS AT  10 11 12 13 14 16 17 18 19 20 21 22 23 24 25 26 27
          28 29 30 31 33 34 35 45 46 47 48 49 50 51 53 54
GGCAT   IS PCY  LOQ  UNS AT  15
GGCAT   IS UNS  AT  33
GGCAT   IS UNS  AT  34
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M1 N   AT  15

```

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 55

## STEREO ATTRIBUTES: NONE

L32 3 SEA FILE=BEILSTEIN SSS FUL L12  
L33 0 SEA FILE=BEILSTEIN SUB=L32 SSS FUL L27

100.0% PROCESSED 3 ITERATIONS  
SEARCH TIME: 00.00.02

0 ANSWERS

# Search history

Berch 10\_716141

12/15/2005

=> d his full

(FILE 'HOME' ENTERED AT 11:24:39 ON 15 DEC 2005)

FILE 'STNGUIDE' ENTERED AT 11:24:46 ON 15 DEC 2005

FILE 'CAPLUS' ENTERED AT 11:24:48 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 11:24:49 ON 15 DEC 2005

L1 STRUCTURE UPLOADED  
L2 1 SEA SSS SAM L1  
D SCA

FILE 'CAPLUS' ENTERED AT 11:28:00 ON 15 DEC 2005

E US2003-716141/APPS  
L3 1 SEA ABB=ON PLU=ON US2003-716141/AP  
SEL RN

FILE 'REGISTRY' ENTERED AT 11:28:58 ON 15 DEC 2005

L4 56 SEA ABB=ON PLU=ON (122-60-1/BI OR 140-18-1/BI OR 309956-78-3/  
BI OR 3355-28-0/BI OR 4403-69-4/BI OR 54249-88-6/BI OR  
666816-91-7/BI OR 666816-98-4/BI OR 668272-43-3/BI OR 668274-18  
-8/BI OR 668276-55-9/BI OR 6971-51-3/BI OR 697806-55-6/BI OR  
697806-56-7/BI OR 697806-57-8/BI OR 697806-58-9/BI OR 697806-59  
-0/BI OR 697806-60-3/BI OR 697806-61-4/BI OR 697806-62-5/BI OR  
697806-63-6/BI OR 697806-64-7/BI OR 697806-65-8/BI OR 697806-66  
-9/BI OR 697806-67-0/BI OR 697806-68-1/BI OR 697806-69-2/BI OR  
697806-70-5/BI OR 697806-71-6/BI OR 697806-72-7/BI OR 697806-73  
-8/BI OR 697806-74-9/BI OR 697806-75-0/BI OR 697806-76-1/BI OR  
697806-77-2/BI OR 697806-78-3/BI OR 697806-79-4/BI OR 697806-80  
-7/BI OR 697806-81-8/BI OR 697806-82-9/BI OR 697806-83-0/BI OR  
697806-84-1/BI OR 697806-85-2/BI OR 697806-86-3/BI OR 697806-87  
-4/BI OR 697806-88-5/BI OR 697806-89-6/BI OR 697806-90-9/BI OR  
697806-91-0/BI OR 697806-92-1/BI OR 697806-93-2/BI OR 697806-94  
-3/BI OR 697806-95-4/BI OR 697806-96-5/BI OR 79-04-9/BI OR  
93703-24-3/BI)  
D SCA

FILE 'LREGISTRY' ENTERED AT 11:30:46 ON 15 DEC 2005

L5 0 SEA SSS FUL L1  
L6 0 SEA SSS SAM L1

FILE 'REGISTRY' ENTERED AT 11:31:25 ON 15 DEC 2005

L7 18 SEA SSS FUL L1  
SAVE TEMP L7 BER141STRA/A

FILE 'CAPLUS' ENTERED AT 11:32:19 ON 15 DEC 2005

L8 2 SEA ABB=ON PLU=ON L7  
L\*\*\* DEL 2 S L4 AND L7

FILE 'REGISTRY' ENTERED AT 11:32:54 ON 15 DEC 2005

L9 6 SEA ABB=ON PLU=ON L4 AND L7  
L10 50 SEA ABB=ON PLU=ON L4 NOT L9  
D SCA

FILE 'STNGUIDE' ENTERED AT 11:36:30 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 14:02:01 ON 15 DEC 2005  
D SCA L7

FILE 'STNGUIDE' ENTERED AT 14:06:18 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 14:53:46 ON 15 DEC 2005  
L11 STRUCTURE UPLOADED

FILE 'STNGUIDE' ENTERED AT 14:54:37 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 14:58:05 ON 15 DEC 2005  
L12 STRUCTURE UPLOADED  
L13 41 SEA SSS SAM L12  
L14 866 SEA SSS FUL L12  
SAVE TEMP BER141STRC/A L14  
L15 38 SEA ABB=ON PLU=ON L4 AND L14  
L16 18 SEA ABB=ON PLU=ON L4 NOT L15  
D SCA

FILE 'STNGUIDE' ENTERED AT 15:03:34 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 15:08:57 ON 15 DEC 2005  
L17 STRUCTURE UPLOADED  
L18 50 SEA SSS SAM L17  
L19 STRUCTURE UPLOADED

FILE 'STNGUIDE' ENTERED AT 15:34:00 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 15:34:48 ON 15 DEC 2005

FILE 'STNGUIDE' ENTERED AT 15:34:52 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 15:37:23 ON 15 DEC 2005  
L20 STRUCTURE UPLOADED  
L21 STRUCTURE UPLOADED  
L22 STRUCTURE UPLOADED  
L23 17 SEA SSS SAM L22  
L24 5 SEA SUB=L14 SSS SAM L22  
D SCA  
L25 72 SEA SUB=L14 SSS FUL L22  
SAVE TEMP L25 BER141STRG/A

FILE 'CAPLUS' ENTERED AT 16:11:18 ON 15 DEC 2005  
L26 7 SEA ABB=ON PLU=ON L25

FILE 'STNGUIDE' ENTERED AT 16:11:50 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 16:20:45 ON 15 DEC 2005

FILE 'STNGUIDE' ENTERED AT 16:20:48 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 16:24:10 ON 15 DEC 2005  
L27 STRUCTURE UPLOADED  
L28 3 SEA SUB=L14 SSS SAM L27  
D SCA  
L29 29 SEA SUB=L14 SSS FUL L27  
D SCA  
SAVE TEMP L29 BER141STRH/A

FILE 'CAPLUS' ENTERED AT 16:33:46 ON 15 DEC 2005  
L30 4 SEA ABB=ON PLU=ON L29

FILE 'BEILSTEIN' ENTERED AT 16:35:09 ON 15 DEC 2005  
L31 0 SEA SSS FUL L27  
L32 3 SEA SSS FUL L12  
L33 0 SEA SUB=L32 SSS FUL L27

FILE 'MARPAT' ENTERED AT 16:37:11 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 16:37:43 ON 15 DEC 2005  
L34 ANALYZE PLU=ON L29 1- LC : 3 TERMS  
D

FILE 'USPATFULL' ENTERED AT 16:38:04 ON 15 DEC 2005  
L35 3 SEA ABB=ON PLU=ON L29

FILE 'STNGUIDE' ENTERED AT 16:40:42 ON 15 DEC 2005

FILE 'REGISTRY' ENTERED AT 16:41:05 ON 15 DEC 2005  
D STAT QUE L29  
D L34

FILE 'CAPLUS' ENTERED AT 16:42:31 ON 15 DEC 2005  
D QUE NOS L30  
D QUE NOS L35

FILE 'REGISTRY' ENTERED AT 16:43:20 ON 15 DEC 2005  
D STAT QUE L29  
D L34

FILE 'CAPLUS' ENTERED AT 16:43:38 ON 15 DEC 2005  
D QUE NOS L30

FILE 'USPATFULL' ENTERED AT 16:43:50 ON 15 DEC 2005  
D QUE NOS L35

FILE 'CAPLUS, USPATFULL' ENTERED AT 16:44:10 ON 15 DEC 2005  
L36 7 DUP REM L30 L35 (0 DUPLICATES REMOVED)  
ANSWERS '1-4' FROM FILE CAPLUS  
ANSWERS '5-7' FROM FILE USPATFULL  
D IBIB ABS HITSTR L36 1-7

FILE 'STNGUIDE' ENTERED AT 16:46:02 ON 15 DEC 2005

FILE 'BEILSTEIN' ENTERED AT 16:46:16 ON 15 DEC 2005  
D STAT QUE L33

FILE 'STNGUIDE' ENTERED AT 16:49:49 ON 15 DEC 2005

FILE HOME

FILE STNGUIDE  
FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Dec 9, 2005 (20051209/UP).

FILE CAPLUS

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FILE COVERS 1907 - 15 Dec 2005 VOL 143 ISS 25  
FILE LAST UPDATED: 14 Dec 2005 (20051214/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

#### FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 DEC 2005 HIGHEST RN 869939-98-0  
DICTIONARY FILE UPDATES: 14 DEC 2005 HIGHEST RN 869939-98-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

#### FILE LREGISTRY

LREGISTRY IS A STATIC LEARNING FILE

NEW CAS INFORMATION USE POLICIES, ENTER HELP USAGETERMS FOR DETAILS.

#### FILE BEILSTEIN

FILE LAST UPDATED ON OCTOBER 10, 2005

FILE COVERS 1771 TO 2005.

**FILE CONTAINS 9,363,954 SUBSTANCES**

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE. \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

NEW

\* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.  
\* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

FILE MARPAT

FILE CONTENT: 1988-PRESENT (VOL 143 ISS 24) (20051211/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES (COVERAGE TO THESE DATES IS NOT COMPLETE):

US 6943267 13 SEP 2005  
DE 1020040544 15 SEP 2005  
EP 1577935 21 SEP 2005  
JP 2005272454 06 OCT 2005  
WO 2005097137 20 OCT 2005

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

MARPATpreviews will be removed from STN on December 31, 2005.

FILE USPATFULL

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 15 Dec 2005 (20051215/PD)  
FILE LAST UPDATED: 15 Dec 2005 (20051215/ED)  
HIGHEST GRANTED PATENT NUMBER: US6976271  
HIGHEST APPLICATION PUBLICATION NUMBER: US2005278816  
CA INDEXING IS CURRENT THROUGH 15 Dec 2005 (20051215/UPCA)  
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 15 Dec 2005 (20051215/PD)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2005  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2005

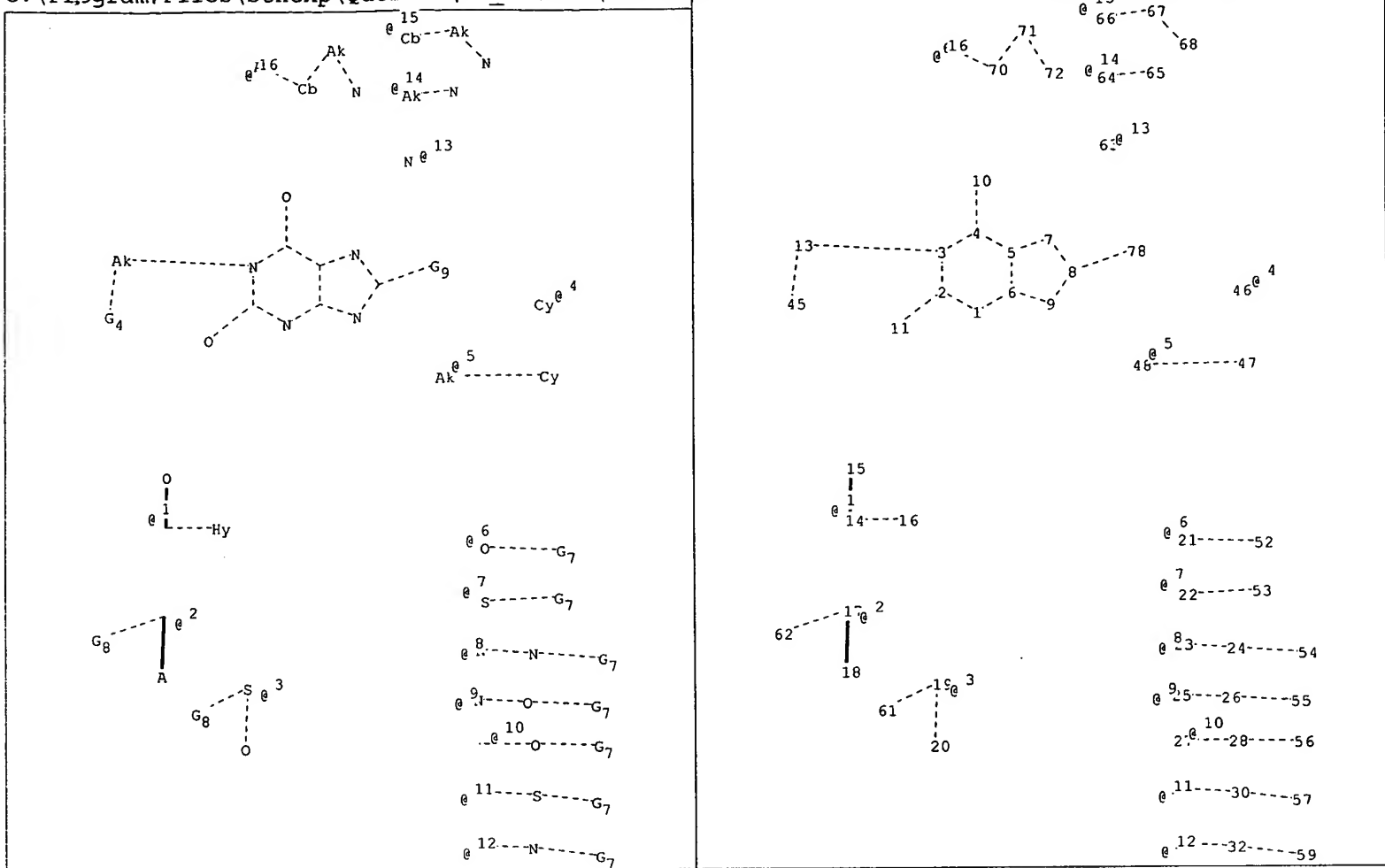
>>> USPAT2 is now available. USPATFULL contains full text of the <<<  
>>> original, i.e., the earliest published granted patents or <<<

>>> applications. USPAT2 contains full text of the latest US <<<  
>>> publications, starting in 2001, for the inventions covered in <<<  
>>> USPATFULL. A USPATFULL record contains not only the original <<<  
>>> published document but also a list of any subsequent <<<  
>>> publications. The publication number, patent kind code, and <<<  
>>> publication date for all the US publications for an invention <<<  
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<  
>>> records and may be searched in standard search fields, e.g., /PN, <<<  
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<  
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<  
>>> enter this cluster. <<<  
>>> <<<  
>>> Use USPATALL when searching terms such as patent assignees, <<<  
>>> classifications, or claims, that may potentially change from <<<  
>>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate  
substance identification.





chain nodes :

10 11 13 14 15 16 20 45 46 47 48 52 53 54 55 56 57 59 64 66 67 69  
70 71 78

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

17 18 19 21 22 23 24 25 26 27 28 29 30 31 32 61 62 63 65 68 72

chain bonds :

2-11 3-13 4-10 8-78 13-45 14-15 14-16 19-20 21-52 22-53 24-54 26-55 28-56  
30-57 32-59 47-48 64-65 66-67 67-68 69-70 70-71 71-72

ring/chain bonds :

17-18 17-62 19-61 23-24 25-26 27-28 29-30 31-32

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-2 1-6 2-3 2-11 3-4 3-13 4-5 4-10 5-6 5-7 6-9 7-8 8-9 8-78 13-45 14-15  
14-16 17-18 17-62 19-20 19-61 21-52 22-53 23-24 24-54 25-26 26-55 27-28 28-56  
29-30 30-57 31-32 32-59 47-48 64-65 66-67 67-68 69-70 70-71 71-72

G4: [\*1], [\*2], [\*3]

G7: [\*4], [\*5]

G8: [\*6], [\*7], [\*8], [\*9], [\*10], [\*11], [\*12]

G9: [\*13], [\*14], [\*15], [\*16]

Connectivity :

2:3 E exact RC ring/chain 4:3 E exact RC ring/chain 9:2 E exact RC ring/chain  
10:1 E exact RC ring/chain 11:1 E exact RC ring/chain 20:1 E exact RC ring/chain

Match level :

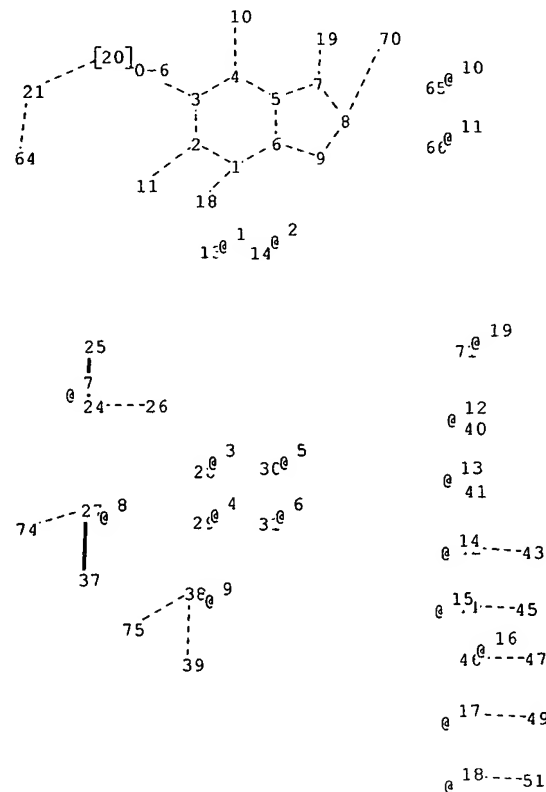
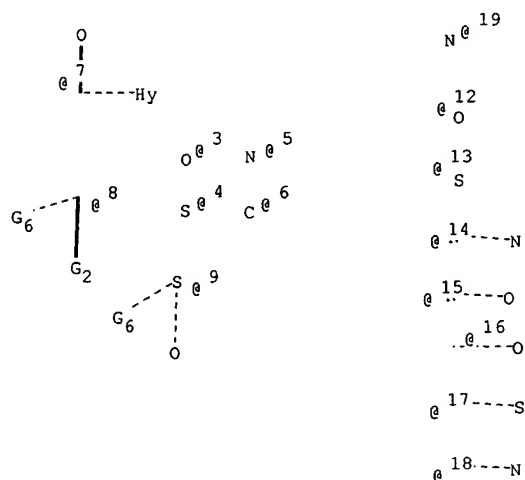
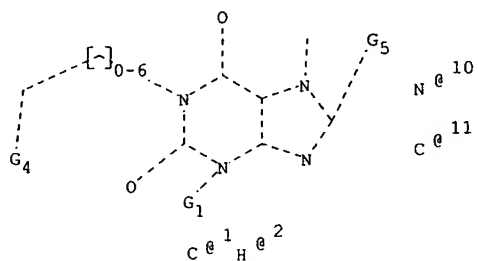
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:CLASS 18:CLASS 19:CLASS 20:CLASS  
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS  
30:CLASS 31:CLASS 32:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 52:CLASS 53:CLASS  
54:CLASS 55:CLASS 56:CLASS 57:CLASS 59:CLASS 61:CLASS 62:CLASS 63:CLASS 64:CLASS  
65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:Atom 71:CLASS 72:CLASS 78:CLASS

Generic attributes :

16:  
Saturation : Unsaturated  
Number of Hetero Atoms : less than 2  
Type of Ring System : Polycyclic  
46:  
Saturation : Unsaturated  
47:  
Saturation : Unsaturated

Element Count :

Node 16: Limited  
N,N1



chain nodes :

10 11 14 18 20 21 24 25 26 39 64 70

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

13 19 27 28 29 30 31 37 38 40 41 42 43 44 45 46 47 48 49 50 51 65  
66 71 74 75

chain bonds :

1-18 2-11 3-20 4-10 7-19 8-70 20-21 21-64 24-25 24-26 38-39

ring/chain bonds :

27-37 27-74 38-75 42-43 44-45 46-47 48-49 50-51

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-2 1-6 1-18 2-3 2-11 3-4 3-20 4-5 4-10 5-6 5-7 6-9 7-8 7-19 8-9 8-70  
20-21 21-64 24-25 24-26 27-37 27-74 38-39 38-75 42-43 44-45 46-47 48-49 50-51

G1: [\*1], [\*2]

G2: [\*3], [\*4], [\*5], [\*6]

G4: [\*7], [\*8], [\*9]

G5: [\*10], [\*11]

G6: [\*12], [\*13], [\*14], [\*15], [\*16], [\*17], [\*18], [\*19]

Connectivity :

2:3 E exact RC ring/chain 4:3 E exact RC ring/chain 9:2 E exact RC ring/chain  
10:1 E exact RC ring/chain 11:1 E exact RC ring/chain 39:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 13:CLASS 14:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 24:CLASS 25:CLASS  
26:Atom 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 37:CLASS 38:CLASS 39:CLASS  
40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS  
49:CLASS 50:CLASS 51:CLASS 64:CLASS 65:CLASS 66:CLASS 70:CLASS 71:CLASS 74:CLASS  
75:CLASS

Generic attributes :

26:  
Saturation : Unsaturated  
Number of Hetero Atoms : less than 2  
Type of Ring System : Polycyclic

Element Count :

Node 26: Limited  
N,N1